Distorting graphene through mechanics and edge chemistry

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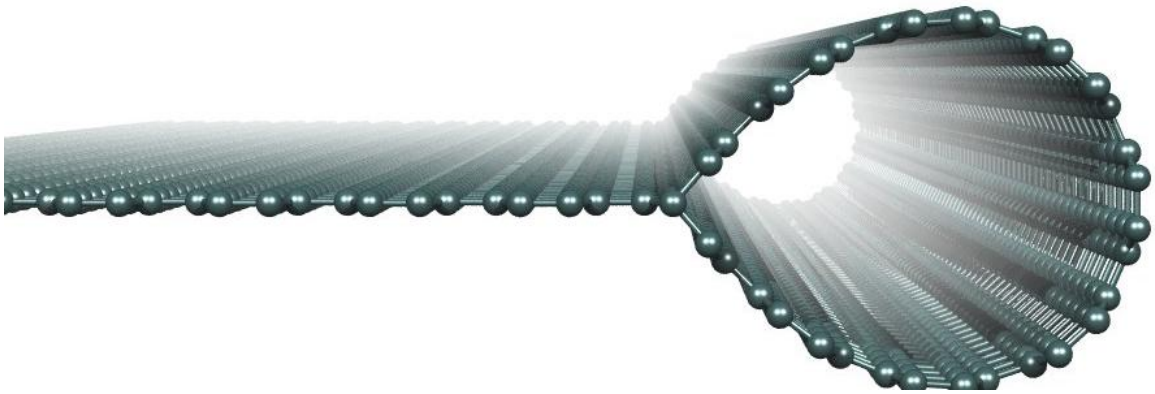
In this talk we consider examples where density functional modelling allows detailed predictions of changes in structural, electronic, mechanical and chemical behaviour of graphene sheets in the presence of intrinsic and extrinsic point and line defects, opening the way to custom design of graphene properties through controlled chemistry.

Interface formation in three-dimensional crystal lattices involves well characterised processes such as rebonding and rehybridisation, localised strain and dislocation formation. In contrast two dimensional crystal lattices, of which graphene is the archetype, are terminated by lines, and the additional available dimension opens up new topological interfacial possibilities. We show via DFT calculations that graphene sheet edges can adopt a range of topological distortions depending on their nature. Rehybridisation, local bond reordering, chemical functionalisation with bulky, charged, or multi-functional groups can lead to edge buckling to relieve strain [1], folding, rolling [2] and even tube formation [3]. As a result careful chemical control of sheet edge functionalisation allows radical modification of ribbon electronic, mechanical and chemical properties, for example reducing the Young's modulus of thinner ribbons by up to 40%.



After one-dimensional strain relief at edges we next examine the importance of lattice strain when considering point defect behaviour, and explore the possibilities for formation and glide of dislocation dipoles at vacancy sites [4]. Finally we show how the mechanical constraints of the graphene lattice can lead to new chemistry, taking the example of gas absorption on graphene surfaces [5].

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